

# Correlation and transport phenomena in topological nodal-loop semimetals

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We study the unique physical properties of topological nodal-loop semimetals protected by the coexistence of time-reversal and inversion symmetries with negligible spin-orbit coupling. We argue that strong correlation effects occur at the surface of such systems for relatively small Hubbard interaction  $U$ , due to the narrow bandwidth of the “drumhead” surface states. In the Hartree-Fock approximation, at small  $U$  we obtain a surface ferromagnetic phase through a continuous quantum phase transition characterized by the surface-mode divergence of the spin susceptibility, while the bulk states remain very robust against local interactions and remain non-ordered. At slightly increased interaction strength, the system quickly changes from a surface ferromagnetic phase to a surface charge-ordered phase through a first-order transition. When Rashba-type spin-orbit coupling is applied to the surface states, a canted ferromagnetic phase occurs at the surface for intermediate values of  $U$ . The quantum critical behavior of the surface ferromagnetic transition is nontrivial in the sense that the surface spin order parameter couple to Fermi-surface excitations from both surface and bulk states. This leads to unconventional Landau damping and consequently a naïve dynamical critical exponent  $z \approx 1$  when the Fermi level is close to the bulk nodal energy. We also show that, already without interactions, quantum oscillations arise due to bulk states, despite the absence of a Fermi surface when the chemical potential is tuned to the energy of the nodal loop. The bulk magnetic susceptibility diverges logarithmically whenever the nodal loop exactly overlaps with a quantized magnetic orbit in the bulk Brillouin zone. These correlation and transport phenomena are unique signatures of nodal loop states.

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The theoretical proposal and experimental verification of Weyl and Dirac semimetals [1–18] has shown that topological electronic structure is not restricted to gapped systems [19–23], but also occurs in gapless systems such as nodal metals[24]. Recently, the interest in topological semimetals has been extended from systems with point nodes to those with a 3D nodal loop, “nodal-chain” [25], “nodal-arc”[26], and even “nodal surfaces” [27], in which there are bulk band touchings along isolated or connected 1D lines, or even at 2D surfaces in the 3D Brillouin zone (BZ) instead of at isolated points.

A growing number of material systems have been theoretically proposed to realize nodal-loop semimetals (NLSMs) [28–36]. In particular, ZrSiS and PbTaSe<sub>2</sub> have been experimentally confirmed by angle-resolved photoemission spectroscopy (ARPES) measurements, and the bulk nodal loops in the ZrSiS-family compounds were further investigated by de Haas-van Alphen (dHvA) quantum oscillations [37, 38] and magneto-transport measurements [39].

In this paper, we discuss some fundamental physics of NLSMs which is distinct from Weyl and Dirac systems. First, we argue that nodal-loop semimetals are prime candidates to observe correlation effects at their surfaces. This is because, unlike point node materials which possess highly dispersive bulk and surface states (typically with large Fermi velocities derived naturally from the several eV width of the associated bands), nodal-loop semimetals possess “drumhead”-like surface states. Depending on surface terminations, the states exist either inside or outside the projection of the nodal loop in the surface BZ.

The dispersion of such drumhead surface states is typically much smaller than that of the bulk valence and conduction bands, raising the interesting possibility of correla-

tion effects occurring at the surface even when interactions are too weak to disturb the electronic states with large kinetic energy in the interior of the sample. Correlations may be induced by Coulomb interactions and/or coupling to phonons, due to the small kinetic energy and large surface density of states. For example, it has been theoretically proposed that such novel flat surface states might support  $s$ -wave superconductivity whose critical temperature scales linearly with the coupling strength [40–42]. Here we argue that repulsive Coulomb interactions generate unusual surface charge density wave and ferromagnetic states, for moderate interaction strength for which the bulk states are unaffected. We expound this in detail through a thorough Hartree-Fock study of a NLSM, including both Hubbard  $U$  and surface Rashba-like spin-orbit coupling (SOC)[43]. This yields a phase diagram showing several correlated surface phases at relatively small values of  $U$ .

Given the prospect for surface quantum phase transitions (QPTs) in these systems, it is interesting to explore the associated quantum critical behavior. We find that such surface QPTs can realize entirely new critical universality classes different from either two or three-dimensional bulk QPTs, owing to their mixed dimensional character. Specifically, a distinct process of Landau damping of order parameter fluctuations into the third dimension arises, and dominates under conditions which we explain.

It is also important to be able to characterize a NLSM by probes other than photoemission, which may be difficult or impossible on many samples, or on appropriate crystal surfaces. In that vein, we derive the existence of unconventional quantum oscillations in NLSMs, which are present even when the Fermi level is exactly at the degeneracy level, so that the system has no true Fermi surface.

These results are expounded in detail in the remainder of the paper, which is organized as follows. In Sec. I, we first a noninteracting tight-binding (TB) model on a tetragonal lattice with both inversion ( $\mathcal{P}$ ) and time-reversal ( $\mathcal{T}$ ) symmetries, which can realize the NLSM phase when spin-orbit coupling (SOC) is neglected. Then, in Sec. II we apply on-site Hubbard interactions (the strength of the interaction is denoted by  $U$ ), and solve such an interacting model in a slab geometry within the Hartree-Fock (HF) approximation, both with and without Rashba SOC, and complement the HF analysis with a study of the susceptibility in the random-phase approximation. Next, in Sec. III, we consider Landau damping of ferromagnetic surface fluctuations, which control quantum critical phenomena [44, 45]. We find in particular that when the Fermi level is close to the nodal energy, the dominant process is one in which an electron-hole pair is shared between the bulk and surface, leading to an unconventional dynamical coefficient  $\sim |\nu_m|q_{\parallel}$  ( $\nu_m$  is the bosonic Matsubara frequency,  $q_{\parallel}$  is the magnitude of in-plane wavevector). This implies a new universality class for the ferromagnetic QPT. Finally, In Sec. IV, we discuss quantum oscillations due to the bulk nodal-loop states, showing that they arise even in the absence of a Fermi surface, and conclude with a summary in Sec. V.

## I. NON-INTERACTING TIGHT-BINDING MODEL

We first construct a non-interacting TB model on a tetragonal lattice with both  $\mathcal{T}$  and  $\mathcal{P}$  symmetries neglecting SOC. As schematically shown in Fig. 1(a), there are two sublattices denoted by  $A$  and  $B$  in each primitive cell, and the hopping from  $A$  to  $B$  along the positive (negative)  $z$  direction is denoted by  $t_1$  ( $t_2$ ). Moreover, there are intra-sublattice in-plane hopping  $t_0$  and inter-sublattice in-plane hopping  $t_3$ . Without the in-plane hoppings, the system can be considered as arrays of decoupled 1D Su-Schrieffer-Heeger (SSH) chains [46, 47]; the in-plane hopping  $t_3$  couple these chains together so that there is band inversion around only one of the eight time-reversal invariant momenta (TRIM). The nodal loop is centered around the TRIM with inverted band order.

The specific properties of the nodal loop such as its size and shape are controlled by  $t_1$ ,  $t_2$  and  $t_3$ , while  $t_0$  renders dispersions to both the bulk nodal energy along the loop and the otherwise flat drumhead surface states. Hereafter we fix  $t_1 = 0.8$ ,  $t_3 = 0.2$ ,  $t_0 = 0.01$ , and  $t_2 > 0$  is the only variable in the noninteracting situation. In particular, when  $t_2 < t_1$ , there is a circular nodal loop centered at the  $X$  ( $(\pi, \pi, \pi)$ ) point. If the surface is truncated at the  $A$  sublattice, one obtains drumhead surface states inside the projected nodal loop centered at  $\bar{X}$  as shown in Fig. 1(b) and Fig. 2(a). If  $t_2 = t_1$ , the nodal loop is diamond-like and connects the TRIM  $X$  and  $M$  ( $(\pi, 0, \pi)$ ). The corresponding surface states fill the region inside the diamond as shown in Fig. 1(c) [48]. When  $t_2 > t_1$ , the nodal loop is centered at  $Z$  ( $(0, 0, \pi)$ ) and the surface states fill the region outside the projected nodal loop (Fig. 1(d) and Fig. 2(b)). It worth to note that for fixed bulk hopping parameters the drumhead surface states can be either inside or outside the projected nodal loop depending on sur-

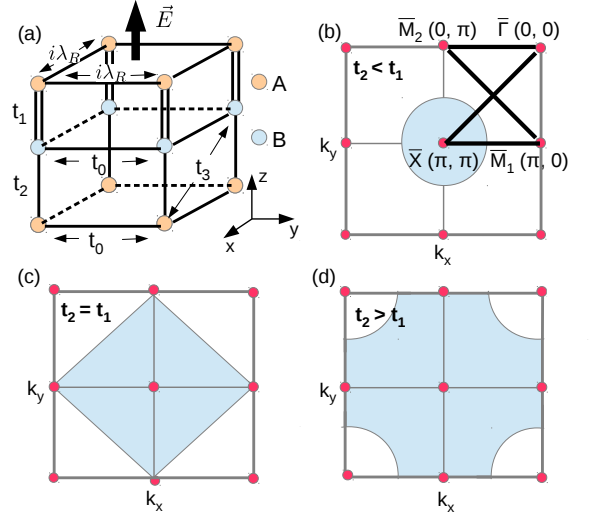


FIG. 1. Schematic illustration of the non-interacting tight-binding model for nodal loop semimetals on a tetragonal lattice. (a) Lattice structure and hopping terms, the thick black arrow indicate surface electric field which generates Rashba SOC denoted by  $\lambda_R$  (b)-(d), nodal loops projected onto the (001) surface BZ, with the shaded region indicating the drumhead surface states, (b) for  $t_2 < t_1$ , (c)  $t_2 = t_1$ , and (d)  $t_2 > t_1$

face terminations (see Appendix C), which is essentially due to the properties of 1D SSH chains. Therefore, the surface states covering a large portion of the surface BZ as shown in Fig. 1(d) can also be realized when  $t_1 < t_2$  if the system is terminated at the other sublattice.

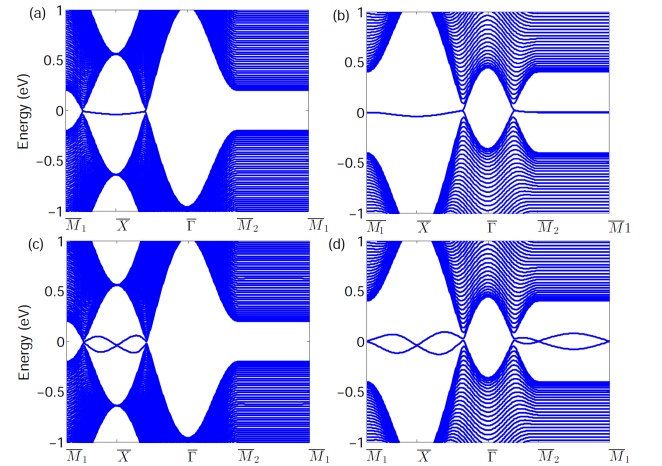


FIG. 2. Surface bandstructures of the non-interacting tight-binding model without surface SOC (a)-(b), and with surface SOC (c)-(d). (a)  $t_2 = 0.75t_1$ , and (b)  $t_2 = 1.25t_1$ ; (c)  $t_2 = 0.75t_1$ ,  $\lambda_R = 0.0625t_1$ , and (d)  $t_2 = 1.25t_1$ ,  $\lambda_R = 0.0625t_1$ . The energy bands are plotted along the high-symmetry path marked by the thick black lines in Fig. 1(b).

Given that inversion symmetry is always broken at a surface, the surface electric field may lead to considerable Rashba spin-orbit splittings in the surface states. Such surface Rashba splittings have been observed in the surfaces of non-

magnetic and magnetic metals [49–51], as well as semiconductor heterostructures [52]. Thus we also take the surface Rashba effects into account by adding a Rashba-type first-neighbor spin-dependent hopping within the surface atomic layer, of which the amplitude is denoted by  $\lambda_R$ . The spin-degenerate drumhead surface states are splitted by such surface SOC (see Fig. 2(c)-(d)); moreover, the surface states acquire nontrivial spin textures. We thus expect that the effects of Coulomb interactions in these two situations (with and without surface SOC) would be different.

## II. EFFECTS OF HUBBARD INTERACTIONS

### A. Without surface Rashba spin-orbit coupling

We first consider the situation without surface Rashba splittings, and apply Hubbard interactions,  $H_U = U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$ , to the above noninteracting tight-binding model in a slab geometry. As the Coulomb interaction at the surface is expected to be strongly screened due to the large surface density of states (DOS), a Hubbard-type local interaction is a good description if we are mainly interested in the effects on the surface states. On the other hand, unlike the surface states of topological insulators, there is no simple low-energy effective Hamiltonian describing the drumhead surface states of NLSMs. Thus we have to construct a slab and apply Hubbard interactions to all the electrons in the slab. Hereafter we will only consider half-filled systems, and we say the system is charge homogeneous with zero charge density if each site is exactly half filled, i.e., there is one electron at each site.

The Hubbard interactions are treated by self-consistent Hartree-Fock (HF) approximation (see Appendix (A) for details). The HF ground states for a slab of 50 primitive cells are shown in Fig. 3(a). When  $U = 0$ , the system is in the NLSM phase. When  $U \sim 10\% - 20\% t_1$ , the system enters into a surface FM (denoted by “surf FM” in the figure) phase with the ferromagnetic order localized at the surface. As  $U$  is further increased, a surface charge-ordered phase becomes energetically favored over the surface FM phase. The system enters into surface CDW phase through a first-order transition. The inset in Fig. 3(a) shows the local charge density along the  $z$  direction for  $U = 0.5t_1$  and  $t_2 = 1.25t_1$ . Clearly the charges are strongly localized at the surface, as the density oscillation decays rapidly into the bulk.

To study the nature of the surface FM transition, we have calculated the spin susceptibility of a 30-unitcell slab in the random phase approximation (RPA) [53] (see Appendix B for details). Fig. 4(a) shows the eigenvalues of static RPA spin susceptibility at different wavevectors at  $U = 0.25t_1$  and  $t_2 = t_1$ . As clearly shown in the figure, there are a large number of quasi-degenerate bands with small amplitudes; moreover, there are two degenerate bands with much larger amplitudes which tend to diverge at  $\Gamma$ . The eigenvectors of the RPA spin susceptibility indicate that those quasi-degenerate bands with small amplitudes are from the bulk spin fluctuations, while the two bands with much larger amplitudes are dominated by acoustic and optical surface fluctuation modes.

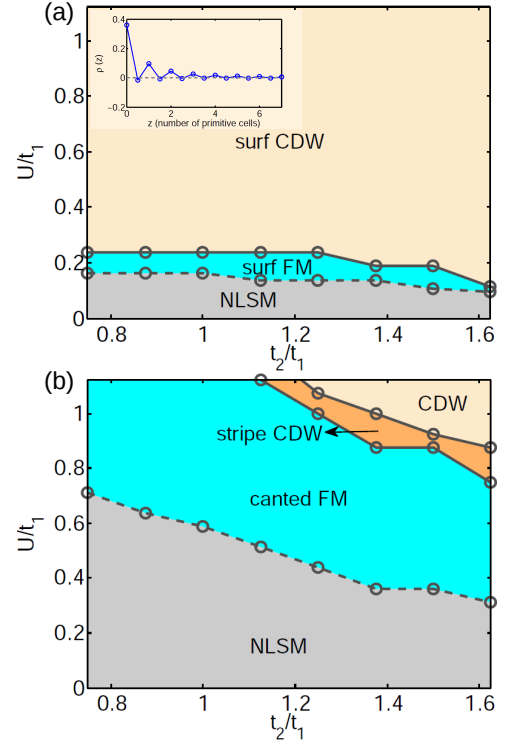


FIG. 3. Phase diagram of the NLSMs with Hubbard interactions in the  $t_2 - U$  parameter space: (a) Without surface Rashba SOC, with the inset shows the local charge density distribution in the surface CDW phase when  $t_2 = 1.25t_1$  and  $U = 0.5t_1$ ; and (b) With surface Rashba SOC.

This is consistent with the expectation that the drumhead surface states are much more sensitive to Coulomb interactions than the bulk states due to the much smaller bandwidth. From Fig. 4(a) it is also evident that the surface spin-fluctuation modes tend to diverge at  $\bar{\Gamma} = (0, 0)$ , indicating a continuous quantum phase transition at the surface driven by Hubbard interactions. We refer the readers to Appendix B for technical details of the implementation of RPA on the slab as well as the properties of the eigenvalues and the eigenvectors of the spin susceptibility.

In Fig. 4(b) we show the parameter dependence of the RPA surface spin susceptibility at  $\bar{\Gamma} = (0, 0)$  (denoted by  $\chi_{zz}^{\text{surf}}(\Gamma)$ ). As is clearly seen from the figure, for a given  $t_2$ , the surface fluctuation modes at  $\bar{\Gamma}$  increase with  $U$ , and diverge at some critical  $U$ , indicating the transition from a nonordered phase to a surface FM phase. The gray dotted line in Fig. 3(b) marks the numeric threshold above which  $\chi_{zz}^{\text{surf}}(\Gamma)$  is considered as diverging. It is interesting to note that as  $t_2$  increases from  $0.75t_1$  (denoted by blue crosses) to  $1.5t_1$  (denoted by cyan diamonds), the critical  $U$  value is reduced by  $\sim 50\%$ . This is because the surface DOS becomes larger for greater  $t_2$  values (Fig. 1(b)-(d)), thus the system becomes more sensitive to Coulomb interactions.

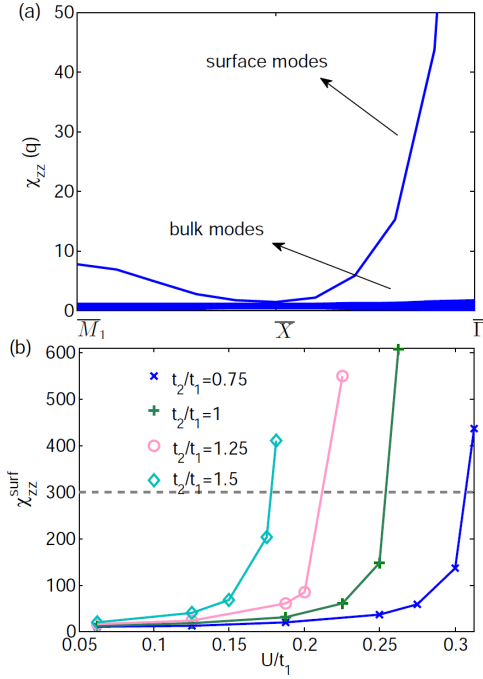


FIG. 4. (a) Dispersion of the spin susceptibility ( $\chi_{zz}(q)$ ) for a 60-layer slab of nodal-loop metal with  $t_2 = t_1$  and  $U = 0.25t_1$ . (b) The  $U$  dependence of the surface spin fluctuations at  $\Gamma$  (denoted by  $\chi_{zz}^{surf}$ ) for different  $t_2$  values.

### B. Hubbard interactions with surface Rashba SOC

We continue to study the effects of Hubbard interactions on NLSMs including surface Rashba splittings with  $\lambda_R = 0.0625t_1$ . Since the surface electric field decays quickly into the bulk, it is assumed that the Rashba SOC  $\lambda_R$  applies only to the topmost and bottommost layers of the slab. The system with such surface SOC expects to be more robust against Coulomb interactions due to the lifted spin degeneracy of the drumhead surface states as shown in Fig. 2(c)-(d). Moreover, as the surface states at the Fermi level acquire nontrivial spin textures due to Rashba SOC, it is unlikely that a charge-ordered phase would be favored.

Both of the above two conjectures are numerically verified as shown in Fig. 3(b). When surface SOC is turned on, our noncollinear self-consistent HF calculations (see Appendix A for technical details) suggest that the system tends to enter into a surface canted FM phase around some moderate  $U$  values ( $U_c \sim 35\% - 65\% t_1$ ). The surface canted FM phase is characterized by ferromagnetically coupled  $z$  components of spins ( $m_z$ ) which are exponentially localized at the surface, and possibly with small spin cantings toward the in-plane directions.

We have also checked the  $U$  dependence of  $m_z$  at the surface layer, and find that  $|m_z|$  increases continuously with  $U$  when  $U \geq U_c$ , indicating a continuous quantum phase transition. The critical value  $U_c$  decreases with the increase of  $t_2$  due to the larger surface DOS for greater  $t_2$  values. The continuous quantum phase transition is further verified by the

divergence of surface spin susceptibility (data not shown). Moreover, it turns out that  $|m_z|$  is likely to have a square root dependence on  $U - U_c$  ( $|m_z| \sim \sqrt{U - U_c}$ ), which is in agreement with the behavior of Stoner ferromagnetism. [54].

When  $t_2 > t_1$  the system tends to go to a surface stripe charge-ordered phase (indicated by “stripe CDW” in Fig. 3(a)) at large  $U$  values, in which there are alternating positive and negative charge stripes along either the  $x$  or the  $y$  direction. There is a transition from such stripe CDW phase to a surface CDW with homogeneous in-plane charge density as  $U$  further increases. Both of these transitions (from canted FM to stripe CDW phase, and from stripe CDW to in-plane homogeneous CDW phase) turn out to be first-order transitions whose phase boundaries are marked by solid lines as shown in Fig. 3(b).

## III. FERROMAGNETIC QUANTUM CRITICALITY AT THE SURFACE

### A. Framework and general considerations

In this section we discuss the quantum critical (QC) behavior near the ferromagnetic transition at the surface of a nodal-loop semimetal neglecting effects of surface SOC. The prototypical description of the quantum phase transition in an itinerant ferromagnet is that of Hertz-Millis theory [44, 45], in which the system is described by an effective action for the order parameter in which the itinerancy of the electrons is reflected by a term representing Landau damping, due to the coupling with Fermi-surface fluctuations [55]. The Landau damping gives rise to a term quadratic in the order parameter with a dynamical coefficient  $\sim |\nu_m|/q$  in the effective action of the spins. Based on this, Hertz derived the dynamical critical exponent  $z = 3$  for FM transitions in 2D and 3D Fermi-liquid systems [44]. The dynamical critical exponent determines the quantum critical phenomenology such as the dependence of critical temperatures on  $U$ , the specific heat, and the crossover behavior from quantum to classical regime at finite temperatures [44, 45]. In two dimensions, there are known flaws in the purely order parameter description, and much theoretical work has gone into improving it [56–58]. Nevertheless, the dynamical scaling  $z \approx 3$  is believed to still be quite a good approximation if not exact.

In NLSMs, we have shown in Sec. II that the FM transition occurs only at the surface and no order occurs in the bulk, so that one may naïvely expect purely two-dimensional FM quantum criticality with  $z \approx 3$ . However, in reality the situation is more complicated due to the gapless bulk states. The electron-hole excitations which couple to the surface spin order parameter arise both from the surface bound states and the extended bulk states, which have an amplitude at the surface. Given the critical role of Landau damping in the theory, we may expect that the quantum critical behavior would be different for such a surface FM transition with gapless bulk excitations.

We confine our analysis here to the level of Landau damping, i.e. the Hertz-Millis order parameter description, which is sufficient to distinguish the difference between purely 2D

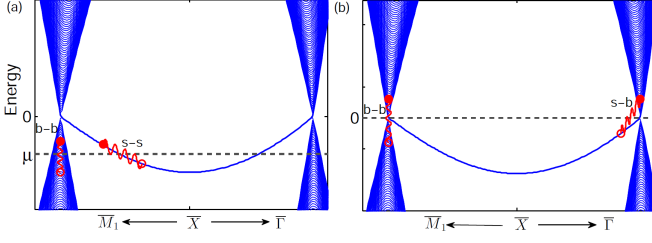


FIG. 5. Schematic illustration of different types of electron-hole excitations that couple to surface spins. (a) When the surface bands are partially filled. (b) When the surface bands are (nearly) completely filled. The electron-hole excitations purely from the surface (bulk) states are denoted by “s-s” (“b-b”); while the process of creating a hole in the surface states and an electron in the bulk states is denoted by “s-b”.

critical behavior and something else. This is already somewhat subtle because several distinct processes may contribute to the damping, i.e. the non-analytic part of the surface spin susceptibility, and one must carefully take into account the momentum and frequency behavior of surface Green’s functions in describing this. It is convenient to decompose the electron-hole excitations into different types. In the first type, both the electron and the hole are created in the surface bound states as denoted by “s-s” in Fig. 5(a); in the second type, that both the electron and the hole are created in the bulk continuum which is denoted as “b-b” in Fig. 5; and finally in the last type, a hole is created in the surface states while an electron is added to the bulk states as denoted by “s-b” in Fig. 5(b).

We consider two different situations. The first situation is that the system is (slightly) hole-doped with partially filled surface bands as schematically shown in Fig. 5(a). In the second situation, the Fermi level is very close to the nodal energy and the drumhead surface states are almost completely filled as sketched in Fig. 5(b). In the first situation we only consider the s-s and b-b type excitations, since the s-b process requires a large momentum transfer, and we are only interested in low-frequency long-wave-length excitations; while in the second case we only consider the s-b and b-b excitations since the surface bands are fully occupied.

## B. Surface Green’s function and Dynamical Susceptibility

We start by calculating the surface Green’s function (SGF) of NLSMs using the method reported in Ref. 59. Note that the SGF includes contributions from both extended and localized eigenstates, and by using an exact method for calculating the SGF, we capture subtle behaviors due to varying contributions of the two types of states. For the tight-binding model given in Sec. I, the surface Green’s function ( $G_s(\mathbf{k}_{\parallel}, \omega)$ ) can be calculated analytically at low energies when the size of the nodal loop is much smaller than that of the BZ. It turns out that the

SGF has a simple analytic solution

$$G_s(\mathbf{k}_{\parallel}, \omega) = \frac{-\tilde{\omega}}{\tilde{t}_1((\sqrt{\gamma^2 - 4} + \gamma)/2 - t_2/\tilde{t}_1)} \approx -\frac{1}{t_2} \frac{\tilde{\omega}}{\sqrt{(k_{\parallel}^2 - k_0^2)^2 - \tilde{\omega}^2 + k_{\parallel}^2 - k_0^2}} \quad (1)$$

where  $\gamma = (\tilde{t}_1^2 + t_2^2 - t_2^2 \tilde{\omega}^2)/(\tilde{t}_1 t_2)$ , and

$$\begin{aligned} \tilde{\omega} &= (\omega - 2t_0(\cos k_x + \cos k_y) + \tilde{\mu})/t_2, \\ &\approx (\omega - (t_0(k_x^2 + k_y^2) - 4t_0) + \tilde{\mu})/t_2, \end{aligned} \quad (2)$$

where  $\tilde{\mu} = \mu/t_2$  with  $\mu$  being the Fermi level, and

$$\begin{aligned} \tilde{t}_1 &= t_1 + 2t_3(\cos k_x + \cos k_y) \\ &\approx t_1 - 4t_2 + t_2(k_x^2 + k_y^2). \end{aligned} \quad (3)$$

We consider the situation that the nodal loop is centered at  $(\pi, \pi, \pi)$  the radius of which is much smaller than the size of the Brillouin zone, and assume that  $t_2 = t_3$ , which is nothing but saying that the bulk Fermi velocity is isotropic. Then the second lines in Eq. (2)-(3) follow by expanding  $\cos k_x$  and  $\cos k_y$  around  $k_x = \pi$  and  $k_y = \pi$ . In Eq. (1)  $k_0$  is introduced as a parameter characterizing the size of the nodal loop:

$$\begin{aligned} \tilde{t}_1 - t_2 &= t_3(k_{\parallel}^2 - k_0^2) \\ &= t_2(k_{\parallel}^2 - k_0^2). \end{aligned} \quad (4)$$

Again, we have assumed that  $t_2 = t_3$  so that the bulk Fermi velocity is isotropic. Starting from Eq. (1) it is straightforward to show that when  $-|k_{\parallel}^2 - k_0^2| \leq \tilde{\omega} \leq |k_{\parallel}^2 - k_0^2|$ ,  $\omega$  is in the bulk gap, and there is a pole at  $\tilde{\omega} = 0$  for  $k_{\parallel} < k_0$  corresponding to the drumhead surface states (the surface is prepared by making a truncation at the  $A$  sublattice); while when  $\tilde{\omega} > |k_{\parallel}^2 - k_0^2|$  or  $\tilde{\omega} < -|k_{\parallel}^2 - k_0^2|$ ,  $\omega$  is in the bulk continuum. Hereafter we will set the bulk nodal energy as 0, so  $\tilde{\omega}$  is shifted by a small constant:  $t_2 \tilde{\omega} = \omega - t_0(k_{\parallel}^2 - k_0^2) + \tilde{\mu}$ . We refer the readers to Appendix C for details in calculating the surface Green’s function.

Eq. (1) may be expressed using the spectral representation as:

$$G_s(\mathbf{k}_{\parallel}, \omega) = \frac{1}{t_2} \int d\epsilon \frac{f(\mathbf{k}_{\parallel}, \epsilon)}{\omega/t_2 - (\epsilon - \tilde{\mu}) + i\delta_{\epsilon}}, \quad (5)$$

where  $\delta_{\epsilon}$  is an infinitesimal quantity which is greater than (less than) zero if  $\epsilon > \tilde{\mu}$  ( $\epsilon < \tilde{\mu}$ ). Or, in the Matsubara formalism,

$$G_s(\mathbf{k}_{\parallel}, i\omega_n) = \frac{1}{t_2} \int d\epsilon \frac{f(\mathbf{k}_{\parallel}, \epsilon)}{i\omega_n/t_2 - (\epsilon - \tilde{\mu})}, \quad (6)$$

The spectral density  $f(\mathbf{k}_{\parallel}, \epsilon)$  consists of two terms:

$$f(\mathbf{k}_{\parallel}, \epsilon) = f_b(\mathbf{k}_{\parallel}, \epsilon) + f_s(\mathbf{k}_{\parallel}, \epsilon). \quad (7)$$

$f_b(\mathbf{k}_{\parallel}, \epsilon)$  is from the bulk continuum, and  $f_s(\mathbf{k}_{\parallel}, \epsilon)$  corresponds to the surface bound state:

$$\begin{aligned} f_b(\mathbf{k}_{\parallel}, \epsilon) &= \frac{\sqrt{(\epsilon - \tilde{t}_0 x_{k_{\parallel}})^2 - x_{k_{\parallel}}^2}}{\epsilon - \tilde{t}_0 x_{k_{\parallel}}} \theta(|\epsilon - \tilde{t}_0 x_{k_{\parallel}}| - |x_{k_{\parallel}}|), \\ f_s(\mathbf{k}_{\parallel}, \epsilon) &= |x_{k_{\parallel}}| \delta(\epsilon - \tilde{t}_0 x_{k_{\parallel}}) \theta(-x_{k_{\parallel}}), \end{aligned} \quad (8)$$



where  $x_{k_{\parallel}} = k_{\parallel}^2 - k_0^2$ , and  $\tilde{t}_0 = t_0/t_2$ .

Now it is straightforward to calculate the dynamical susceptibility using the surface Green's function shown in Eq. (5)-(8). To be specific, using the Matsubara formalism, the dynamical susceptibility is expressed as:

$$\chi(\mathbf{q}_{\parallel}, i\nu_m) = -\frac{1}{\beta} \int_{\mathbf{k}_{\parallel}} \sum_n G_s(\mathbf{k}_{\parallel}, i\omega_n) G_s(\mathbf{k}_{\parallel} + \mathbf{q}_{\parallel}, i\omega_n + i\nu_m). \quad (9)$$

where  $\int_{\mathbf{k}_{\parallel}} = \int dk_x dk_y / (2\pi)^2$ ,  $\beta = 1/(k_B T)$  is the inverse temperature, and  $(\mathbf{k}, \omega)$  and  $(\mathbf{q}, \nu)$  denote Fermionic and Bosonic wavevectors and frequencies respectively.  $\mathbf{k}_{\parallel}$  ( $\mathbf{q}_{\parallel}$ ) represents an in-plane wavevector. Plugging Eq. (5) in to Eq. (9), and summing over the Matsubara frequencies using the standard contour technique, then taking the analytic continuation  $i\nu_m \rightarrow \nu + i\delta$ , one obtains

$$\text{Im } \chi(\mathbf{q}_{\parallel}, \nu, \mu) = \int_{\mathbf{k}_{\parallel}} \int_{-\tilde{\mu}}^{-\tilde{\mu}+\tilde{\nu}} \frac{d\epsilon}{t_2} f(-\epsilon, \mathbf{k}_{\parallel}) f(\tilde{\nu} - \epsilon, \mathbf{k}_{\parallel} + \mathbf{q}_{\parallel}) \quad (10)$$

where  $\tilde{\mu} = \mu/t_2$ , and  $\tilde{\nu} = \nu/t_2$ , with  $\mu$  being the Fermi level. Since  $f = f_s + f_b$ ,  $\chi(\mathbf{q}_{\parallel}, \nu)$  can be decomposed into four terms which are the bulk-bulk ( $\chi_{bb}$ ), surface-bulk ( $\chi_{sb}$ ), bulk-surface ( $\chi_{bs}$ ) and surface-surface ( $\chi_{ss}$ ) contributions. We will discuss these contributions separately in the following paragraphs.

### C. Partially filled surface bands

Let us first consider the situation with partially filled surface bands as shown in Fig. 5(a) with  $\mu < 0$ . The dynamical susceptibility contributed by the  $s-s$  process (denoted by  $\chi_{ss}(\mathbf{q}_{\parallel}, \nu)$ ) behaves similarly to the 2D Linhard function because the SGF has a pole at  $\tilde{\omega} = 0$  for  $k_{\parallel} < k_0$ , which looks similar to that of 2D free electrons with quadratic dispersion. Thus the imaginary part of zero-temperature susceptibility  $\text{Im } \chi_{ss}(\mathbf{q}_{\parallel}, \nu) \sim \nu/q_{\parallel}$  at small in-plane wavevector  $q_{\parallel}$  and low frequency  $\nu \ll \hbar v_F^s q_{\parallel}$  with  $v_F^s$  referring to the Fermi velocity of the surface bands (In the finite-temperature formalism  $\chi_{ss}(\mathbf{q}_{\parallel}, \nu_m) \sim |\nu_m|/q_{\parallel}$  with  $\nu_m$  being Bosonic Matsubara frequency.). On the other hand, the dynamical susceptibility contributed by the  $b-b$  process  $\chi_{bb}(\mathbf{q}_{\parallel}, \nu)$  with  $|\nu| < |\mu|$  is expressed as:

$$\text{Im } \chi_{bb}(\mathbf{q}_{\parallel}, \nu, \mu) = \int_{\mathbf{k}_{\parallel}} \int_{-\tilde{\mu}}^{-\tilde{\mu}+\tilde{\nu}} \frac{d\epsilon}{t_2} f_b(-\epsilon, \mathbf{k}_{\parallel}) f_b(\nu - \epsilon, \mathbf{k}_{\parallel} + \mathbf{q}_{\parallel}), \quad (11)$$

After some algebra, it turns out that when  $\nu \ll \hbar v_F q_{\parallel}$  ( $v_F$  is the bulk Fermi velocity):

$$\text{Im } \chi_{bb}(\mathbf{q}_{\parallel}, \nu, \mu) \sim \frac{\nu}{q_{\parallel}}. \quad (12)$$

Therefore  $\chi_{bb}$  is equally important as  $\chi_{ss}$  for the hole-doped case. In other words, the dominant Landau damping is from both the surface and the bulk, and they make comparable contributions. Thus we expect the usual theory of 2d FM quantum critical still applies, with consequently dynamical critical exponent  $z \approx 3$ . It is also interesting to note that as a result of

the fluctuations in the third spatial dimension,  $\chi_{bb}(\mathbf{q}_{\parallel}, \nu)$  is nonvanishing even when  $q_{\parallel} = 0$ . It turns out that

$$\text{Im } \chi_{bb}(q_{\parallel} = 0, \nu, \mu) \sim \nu, \quad (13)$$

which is unusual for a ferromagnetic phase transition. We refer the readers to Appendix D for the derivations of Eq. (12) and Eq. (13).

The analytic results shown in Eq. (11) and Eq. (13) are supported by direct numeric calculations of the surface dynamical susceptibility of a 500-cell slab of the tight-binding model introduced in Sec. I. The Fermi level  $\mu = -0.036$  as schematically indicated by the gray dashed line in Fig. 5(a),  $t_0 = 0.01$ ,  $t_1 = 0.8$ ,  $t_2 = 0.3$  and  $t_3 = 0.2$ . The frequency dependence of surface dynamical susceptibility at  $q_{\parallel} = 0$  is shown in Fig. 6(a). Clearly at low frequencies,  $\chi_{bb}(0, \nu)$  is linear in  $\nu$ , in agreement with Eq. (13).

We also study the wavevector dependence of  $\chi_{bb}(\mathbf{q}_{\parallel}, \nu)$  for a given frequency  $\nu = 0.008$  as shown in Fig. 6(b).  $\text{Im } \chi_{bb}(\mathbf{q}_{\parallel}, \nu)$  is linearly dependent on  $1/q_x$  for  $0.065 \lesssim q_{\parallel} \lesssim 0.085$  (in units of  $1/a$ , where  $a = 1$  is the in-plane lattice constant). When  $q_{\parallel} \lesssim 0.06$ , we are no longer in the regime that  $\nu \ll \hbar v_F q_{\parallel}$  and in the meanwhile  $1/q_{\parallel}$  becomes comparable to the  $\mathbf{k}$ -mesh density, so that Eq. (12) is no longer valid; while when  $q_{\parallel}$  is large ( $q_{\parallel} \gtrsim 0.085$ ), the wavevector becomes comparable to the radius of the bulk ‘‘Dirac cone’’ above which the electron-hole excitations are rigorously truncated. This explains why the  $1/q_{\parallel}$  behavior is observed only for  $0.065 \lesssim q_{\parallel} \lesssim 0.086$ . The details of computing the surface dynamical susceptibility is explained in Appendix E.

### D. Nearly full surface bands

We continue studying the case when the surface bands are nearly completely filled as shown in Fig. 5(b). In such a situation, the Fermi level  $\mu = 0$ , and the dominating contribution is either  $b-b$  or  $s-b$  process. The surface dynamical susceptibility from the  $s-b$  process is expressed as

$$\text{Im } \chi_{sb}(\mathbf{q}_{\parallel}, \nu, \mu = 0) = \int_{\mathbf{k}_{\parallel}} \int_0^{\tilde{\nu}} \frac{d\epsilon}{t_2} f_s(-\epsilon, \mathbf{k}_{\parallel}) f_b(\nu - \epsilon, \mathbf{k}_{\parallel} + \mathbf{q}_{\parallel}), \quad (14)$$

and the  $b-b$  contribution is expressed in Eq. (11) with  $\mu = 0$ . After solving these integrals, it turns out that

$$\text{Im } \chi_{bb}(\mathbf{q}_{\parallel}, \nu, \mu = 0) \sim \nu^3/q_{\parallel}, \quad (15)$$

$$\text{Im } \chi_{sb}(\mathbf{q}_{\parallel}, \nu, \mu = 0) \sim q_{\parallel}(\nu - \eta(t_0, q_{\parallel})), \quad (16)$$

where  $\eta(t_0, q_{\parallel}) = 2t_0(2k_0 q_{\parallel} - q_{\parallel}^2)/3$  is the energy gap of the  $s-b$  particle-hole excitations. Physically Eq. (16) implies that a minimal frequency  $\sim \eta(t_0, q_{\parallel})$  is required to create an electron-hole pair of the  $s-b$  type with finite wavevector  $q_{\parallel}$ . Such a minimal excitation energy  $\sim t_0$ , and vanishes when the surface bands are perfectly flat (remember that the surface bandwidth arises due to  $t_0$ ) or when  $q_{\parallel} \rightarrow 0$ . We refer the readers to Appendix D for the derivations of Eq. (15)-(16).

Eq. (15)-(16) indicate that when  $\mu = 0$  the  $s-b$  process dominates over the  $b-b$  process at low frequencies and

TABLE I. Linear fits to the frequency dependence of surface susceptibility at different wavevectors

$q_{  }$	0.4	0.3	0.25	0.2	0.15	0.1	0.05
$c$	0.6075	0.5099	0.4536	0.3892	0.3143	0.2294	0.1377
$\eta(t_0, q_{  })$	0.0054	0.0041	0.0036	0.0030	0.0025	0.0017	0.0014

small wavevectors. If we follow the Hertz-Millis procedure, a straightforward analysis then predicts the dynamical critical exponent  $z \approx 1$ . Subtleties similar to those in the purely 2D case may still occur here, of course, but this result is sufficient to show that the quantum critical behavior at this transition is fundamentally different from that of a purely 2D itinerant ferromagnet. We once again note that, when  $q_{||} = 0$ ,  $\text{Im } \chi_{bb}(0, \nu)$  is non-vanishing and  $\sim \nu^2$  for  $\mu = 0$  due to the Fermionic fluctuations in the  $z$  direction.

Again, the analytic results in Eq. (15)-(16) are numerically verified by directly computing the surface-layer dynamical susceptibility of a 500-cell slab. The Fermi level is very close to the nodal loop in the calculations as indicated by the gray dashed line in Fig. 5(b). The surface bound states are almost completely filled. The other parameters of the tight-binding model are the same as those in the previous susceptibility calculation. The frequency dependence of the surface susceptibility at  $q_{||} = 0.4$  (denoted by  $\text{Im } \chi_{sb}(0.4, \nu)$ ) is shown in Fig. 7(a). Clearly  $\text{Im } \chi_{sb}(0.4, \nu) \sim \nu$  at low frequencies and there is a small energy gap around  $\nu \sim t_0$ , in agreement with Eq. (16).

In order to study the wavevector dependence of the energy gap  $\eta(t_0, q_{||})$ , we have calculated the frequency dependence of the surface dynamical susceptibility of a 500-cell slab for different wavevectors from  $q_{||} = 0.4$  to  $q_{||} = 0.05$ . Then we fit the data with linear functions  $y = c(x - \eta(t_0, q_{||}))$  ( $y$  is  $\text{Im } \chi_{sb}(q_{||}, \nu)$ ,  $x$  is  $\nu$ ). The parameters  $c$ s and  $\eta(t_0, q_{||})$ s are shown in Table I. As clearly shown in the table,  $\eta(t_0, q_{||})$  decreases with  $q_{||}$  and tend to vanish as  $q_{||} \rightarrow 0$  [60].

We also numerically calculate the wavevector dependence of the surface dynamical susceptibility at  $\nu = 0.025$  as shown in Fig. 7(b). Clearly  $\text{Im } \chi_{sb}(q_{||}, 0.025) \sim q_{||}$  at small  $q_{||}$ , in agreement with the analytic prediction of Eq. (16). It should be noted that when the Fermi level is at the nodal energy, the  $b-b$  process is suppressed at relatively large wavevector ( $q_{||} \gtrsim 0.05$ ), thus the data shown in Fig. 7(a)-(b) is mostly contributed by  $s-b$  process. We refer the readers to Appendix E for details in the the numeric calculations of surface dynamical susceptibility.

#### IV. BULK QUANTUM OSCILLATIONS

We turn to discussing the bulk quantum oscillations of NLSMs neglecting Coulomb interactions. We introduce the following low-energy effective Hamiltonians describing nodal

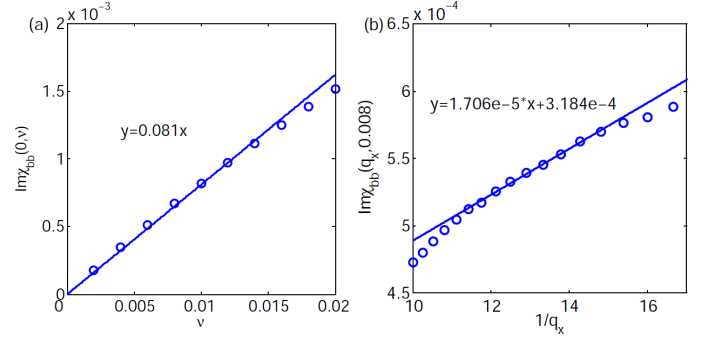


FIG. 6. Numerical calculations of the surface dynamical susceptibility of slightly hole-doped nodal-loop semimetals with partially filled surface bands: (a) frequency dependence at  $q_{||} = 0$ ; and (b) wavevector dependence at  $\nu = 0.008$ . Note the horizontal axis in (b) is  $1/q_x$ .

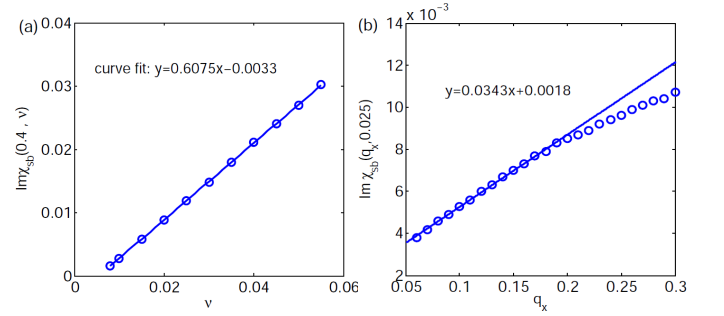


FIG. 7. Numerical calculations of the surface dynamical susceptibility of charge neutral nodal-loop semimetals with nearly completely filled surface bands: (a) the frequency dependence at  $q_{||} = 0.4$ , and (b) the wavevector dependence at  $\nu = 0.025$ .

loops with different in-plane dispersions:

$$H_0^{\text{qua}} = \hbar v_z k_z \sigma_y + \left( \Delta - \frac{\hbar^2 (k_x^2 + k_y^2)}{2m} \right) \sigma_z$$

$$H_0^{\text{lin}} = \hbar v_z k_z \sigma_y + \left( \Delta - \hbar v_0 \sqrt{k_x^2 + k_y^2} \right) \sigma_z, \quad (17)$$

where  $\sigma_y$  and  $\sigma_z$  are the Pauli matrices representing the lowest conduction band and highest valence band at some high-symmetry point ( $\mathbf{k} = (0, 0, 0)$ ),  $v_z$  is the Fermi velocity along the  $z$  direction, and  $\Delta$  is the gap at  $\mathbf{k} = (0, 0, 0)$ .  $H_0^{\text{qua}}$  describes a circular nodal loop with quadratic in-plane dispersion, of which the in-plane effective mass is denoted by  $m$ ; while  $H_0^{\text{lin}}$  describes a nodal loop with linear in-plane dispersion with in-plane Fermi velocity  $v_0$ . The nodal energies described by Eq. (17) are exactly zeros.

The Landau levels for the above two effective Hamiltonians with  $\mathbf{B} = B \hat{e}_z$  are readily obtained:

$$E_{\pm}^{\text{qua}}(n, k_z) = \pm \sqrt{(\Delta - \hbar \omega_c (n + 1/2))^2 + \hbar v^2 k_z^2}$$

$$E_{\pm}^{\text{lin}}(n, k_z) = \pm \sqrt{(\Delta - \hbar \omega_c \sqrt{n + 1/2})^2 + \hbar v^2 k_z^2}, \quad (18)$$

where the cyclotron frequency

$$\omega_c = \begin{cases} eB/m & \text{for quadratic in-plane dispersion} \\ \sqrt{2eBv_0^2/\hbar} & \text{for linear in-plane dispersion} \end{cases} \quad (19)$$

for the case of linear dispersion. If the chemical potential is exactly at the nodal energy, i.e.,  $\mu = 0$ , in general the Landau level spectrum is gapped and the chemical potential is in the middle of the gap. However, the gap closes at  $k_z = 0$  whenever  $\Delta = \hbar\omega_c(n + 1/2)$  for quadratic in-plane dispersion, and  $\Delta = \hbar\omega_c\sqrt{(n + 1/2)}$  for linear in-plane dispersion. Note that the above gap-closure condition is nothing but the equality between the area of the nodal loop  $\mathcal{A}_{\text{NL}}$  and the area of the  $n$ th quantized magnetic orbit  $\mathcal{A}_{\text{B}}(n)$ , i.e.,  $\mathcal{A}_{\text{NL}} = \mathcal{A}_{\text{B}}(n)$ , where  $\mathcal{A}_{\text{NL}} = \pi\Delta^2/(\hbar^2v_0^2)$  ( $\mathcal{A}_{\text{NL}} = 2\pi m\Delta/(\hbar^2)$ ) for a nodal loop with linear (quadratic) in-plane dispersions, and the area of  $n$ th magnetic orbit  $\mathcal{A}_{\text{B}}(n) = 2\pi eB(n + 1/2)/\hbar$ .

In other words, the Landau levels become gapless whenever the nodal loop exactly overlaps with a quantized magnetic orbit. At the gapless point there expects to be a sharp change in the free energy because a fully occupied Landau level becomes completely unoccupied due to the gap closure and reopening. Thus some singular behavior is expected at the gapless critical point.

To confirm the above conjecture, we calculate the magnetic susceptibility  $\chi(B) = -\partial^2 F/\partial B^2$  for the Landau levels shown in Eq. (18) in the limit  $\mu \rightarrow 0$  and  $T \rightarrow 0$ . It turns out that the magnetic susceptibility consists a term which diverge logarithmically when the Landau level is gapless:

$$\lim_{\mu \rightarrow 0, T \rightarrow 0} \chi(B) \sim \frac{e^2\omega_c}{\pi^2\hbar m v_z} \sum_{n=0}^{\infty} (n + 1/2)^2 \times \ln \left( \frac{\sqrt{(\Delta/\omega_c - (n + 1/2))^2 + \Lambda^2} + \Lambda}{|\Delta/\omega_c - (n + 1/2)|} \right) \quad (20)$$

for quadratic-inplane dispersion, and

$$\lim_{\mu \rightarrow 0, T \rightarrow 0} \chi(B) \sim \frac{eB}{2\pi^2\hbar} \frac{e^2v_0^4}{\omega_c^2} \frac{2\Delta}{\omega_c v_z} \sum_{n=0}^{\infty} \sqrt{n + 1/2} \times \ln \left( \frac{\sqrt{(\Delta/\omega_c - \sqrt{n + 1/2})^2 + \Lambda^2} + \Lambda}{|\Delta/\omega_c - \sqrt{n + 1/2}|} \right) \quad (21)$$

for linear in-plane dispersion, where  $\Lambda = (\pi v_z)/(\omega_c a)$  is a cutoff parameter with  $a$  being the lattice constant on the order of 1 Å. Such logarithmic divergence indicates a magnetic-field-driven quantum phase transitions in NLSMs [61]. More detailed results about the dHvA quantum oscillations of NLSMs are presented in Supplementary Material.

## V. CONCLUSION

To summarize, we have studied the effects of Hubbard interactions and bulk quantum oscillations in NLSMs. Our

HF calculations indicate that Hubbard interactions tend to drive the system into surface-ordered phases through quantum phase transitions at the surface. In particular, in the absence of surface Rashba SOC, the system becomes ferromagnetic at the surface at small  $U$ , and enters into a surface charge-ordered phase at slightly increased  $U$  through a first-order transition. On the other hand, surface Rashba SOC splits the otherwise two-fold degenerate drumhead surface states and endows them with nontrivial spin textures, so that a surface canted FM phase becomes stable for moderate  $U$  values. The quantum critical behavior of the surface ferromagnetic transition is distinct from that in conventional 2D or 3D metals. This is due to novel Landau damping of the 2D spin fluctuations into electron-hole excitations near the nodal loop in the third dimension. This “mixed dimensionality” of the system is argued to result in a modified dynamical critical exponent, with  $z \approx 1$  at the level of a Hertz-Millis analysis, when the Fermi level is close to the bulk nodal energy. We have also studied the bulk quantum oscillations of NLSMs in the non-interacting case, and find that in the limit of zero temperature and zero chemical potential, there is a logarithmic divergence in the magnetic susceptibility whenever the nodal loop overlaps with a quantized magnetic orbit. Such a logarithmic divergence is accompanied by the gap closure of the Landau levels, and is periodic in  $1/B$ . The predictions of interaction-driven surface ordering and novel bulk quantum oscillations may stimulate future experimental and theoretical studies of NLSMs.

*Note added.* Recently we became aware of two related works by H. K. Pal *et al.* [62] and B. Roy [63]. In the former, the authors have thoroughly studied the quantum-oscillation behaviors of various physical quantities in a model of two dimensional valence and conduction bands that touch along a loop, and in this context explored the temperature dependence of the quantum oscillations. In the latter, the author has discussed effects of Coulomb interactions in the bulk of nodal-loop semimetals.

## ACKNOWLEDGMENTS

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## Appendix A: Self-consistent Hartree-Fock approximation

In Sec. II, the self-consistent Hartree-Fock (HF) approximation is adopted to calculate the ground states of the interacting Hamiltonians, i.e.,

$$U\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} \rightarrow U\langle\hat{n}_{i\uparrow}\rangle\hat{n}_{i\downarrow} + U\hat{n}_{i\uparrow}\langle\hat{n}_{i\downarrow}\rangle - U\langle\hat{n}_{i\uparrow}\rangle\langle\hat{n}_{i\downarrow}\rangle \quad (\text{A1})$$

where  $\hat{n}_{i\sigma}$  refers to the density operator of electrons with spin  $\sigma$  ( $\sigma = \uparrow, \downarrow$ ) at site  $i$ ,  $\langle\hat{n}_{i\sigma}\rangle$  is the self-consistent mean field applied to the electrons of spin  $-\sigma$  at site  $i$ ;  $U$  denotes the amplitude of the Hubbard repulsion. The linear tetrahedron method



[64] is implemented as an interpolation scheme so that the self-consistent calculations can be carried out with improved numeric efficiency.

Including SOC, the noncollinear HF is slightly more complicated than its collinear version:

$$Un_{i\uparrow}n_{i\downarrow} \rightarrow U[c_{i\uparrow}^\dagger, c_{i\downarrow}^\dagger](\langle n_i \rangle - \mathbf{m}_i \cdot \mathbf{s}_i)[c_{i\uparrow}, c_{i\downarrow}]^T - U\langle n_{i\uparrow} \rangle \langle n_{i\downarrow} \rangle + U\langle c_{i\uparrow}^\dagger c_{i\downarrow} \rangle \langle c_{i\downarrow}^\dagger c_{i\uparrow} \rangle, \quad (\text{A2})$$

where  $c_{i\uparrow(\downarrow)}^\dagger$  ( $c_{i\uparrow(\downarrow)}$ ) represents the creation (annihilation) operator of electrons at site  $i$  with  $\uparrow(\downarrow)$  denoting electrons' spins.  $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$  ( $\sigma = \uparrow, \downarrow$ ) is the number operator at site  $i$  with spin  $\sigma$ , and  $n_i = n_{i\uparrow} + n_{i\downarrow}$  is the total number operator.  $\langle \dots \rangle$  represents the expectation value of some operator in the HF ground state.  $\mathbf{s}_i = [s_i^x, s_i^y, s_i^z]$  are the Pauli matrices representing an electron's spin at site  $i$ , which couples to the self-consistent vector field  $\mathbf{m}_i = [m_i^x, m_i^y, m_i^z]$ , where

$$\begin{aligned} m_i^x &= \langle c_{i\uparrow}^\dagger c_{i\downarrow} + c_{i\downarrow}^\dagger c_{i\uparrow} \rangle \\ m_i^y &= i\langle c_{i\downarrow}^\dagger c_{i\uparrow} - c_{i\uparrow}^\dagger c_{i\downarrow} \rangle \\ m_i^z &= \langle c_{i\uparrow}^\dagger c_{i\uparrow} - c_{i\downarrow}^\dagger c_{i\downarrow} \rangle \end{aligned} \quad (\text{A3})$$

## Appendix B: Generalized RPA susceptibility

The generalized susceptibility in the random phase approximation (RPA)  $\chi^{\text{RPA}}$  can be expressed as [53]

$$\chi^{\text{RPA}} = (1 - \chi^{(0)}\mathbb{U})^{-1}\chi^{(0)} \quad (\text{B1})$$

where  $\chi^{(0)}$  and  $\mathbb{U}$  are the matrices representing the bare susceptibility and the Coulomb interactions respectively. To be specific, the bare susceptibility can be calculated from the noninteracting Green's function,

$$\chi_{\alpha\beta l, \alpha'\beta' l'}^{(0)}(\mathbf{q}, i\nu_n) = -k_B T \int \frac{dk^2}{(2\pi)^2} \sum_{i\omega_n} G_{\alpha' l', \alpha l}^{(0)}(\mathbf{k}, i\omega_n) \times G_{\beta l, \beta' l'}^{(0)}(\mathbf{k} + \mathbf{q}, i\omega_n + i\nu_n), \quad (\text{B2})$$

where the  $\alpha, \alpha', \beta$  and  $\beta'$  are the spin indices, while  $l$  and  $l'$  label the lattice sites in the slab;  $\mathbf{k}$  is the wavevector of the noninteracting Bloch functions, and the sum over Matsubara frequency  $\omega_n$  can be taken analytically in the basis that diagonalizes the noninteracting Hamiltonian at each  $\mathbf{k}$ .  $k_B$  is the Boltzman constant and  $T$  is the temperature;  $k_B T$  is fixed as 1/100 in the RPA calculations in Sec. II. Note that in the nonordered phase without spin-orbit coupling, all kinds of spin fluctuations are equivalent to each other, i.e.,  $\chi_{\uparrow\uparrow l, \uparrow\uparrow l'}^{(0)} = \chi_{\uparrow\uparrow l, \uparrow\downarrow l'}^{(0)} = \chi_{\uparrow\downarrow l, \uparrow\uparrow l'}^{(0)} = \chi_{\uparrow\downarrow l, \uparrow\downarrow l'}^{(0)}$ . With SOC included, terms like  $\chi_{\uparrow\uparrow l, \downarrow\downarrow l'}^{(0)}$  are also allowed, and spin fluctuations become anisotropic.

The interaction matrix for Hubbard interactions is defined as:

$$\mathbb{U}_{\beta\alpha', \alpha\beta'}^{l, l'} = -(U\delta_{l, l'}\delta_{\beta'\alpha'}\delta_{\beta\alpha}\delta_{\alpha, -\alpha'} - U\delta_{l, l'}\delta_{\alpha\beta'}\delta_{\beta\alpha'}\delta_{\alpha, -\beta}) \quad (\text{B3})$$

The over minus sign on the right-hand-side (RHS) of Eq. (B3) is from the minus sign in the time-ordered exponential of the  $S$  matrix [54]. The first term on the RHS of Eq. (B3) represents a direct Coulomb interaction, while the second term is the exchange interaction. Then the matrix element of the static RPA spin susceptibility ( $\chi_{zz}^{\text{RPA}}(\mathbf{q})$ ) is expressed as

$$\begin{aligned} \chi_{zz}^{\text{RPA}}(\mathbf{q})_{l, l'} &= \chi^{\text{RPA}}(\mathbf{q})_{\uparrow\uparrow l, \uparrow\uparrow l'} - \chi^{\text{RPA}}(\mathbf{q})_{\downarrow\downarrow l, \uparrow\uparrow l'} - \\ &\quad \chi^{\text{RPA}}(\mathbf{q})_{\uparrow\uparrow l, \downarrow\downarrow l'} + \chi^{\text{RPA}}(\mathbf{q})_{\downarrow\downarrow l, \downarrow\downarrow l'} \end{aligned} \quad (\text{B4})$$

The eigenvalues of the RPA spin susceptibility at  $t_2 = t_1$  and  $U = 0.25t_1$  ( $t_1$  and  $t_2$  are defined in Sec. I) are shown in Fig. 4(a). As discussed in Sec. II, the surface modes are much stronger than the bulk modes, and tend to diverge at  $\bar{\Gamma}$  as  $U$  approaches some critical value  $U_c$  indicating a continuous quantum phase transition at the surface.

## Appendix C: Surface Green's function

In this section we derive the surface Green's function of NLSMs using the method reported in Ref. 59. To be specific, using the Dyson equation, the surface Green's function  $G_s(\mathbf{k}_{\parallel}, \omega)$  can be expressed as:

$$G_s = G_0 + G_0 V G_s, \quad (\text{C1})$$

where  $G_s$  is the full surface Green's function with the corresponding Hamiltonian  $H$ ,  $V = H - H_0$  is the potential difference between a crystal with and without a surface, and  $G_0$  is the noninteracting bulk Green's function. In the basis of the "hybrid Wannier functions" [65] which are extended in the  $x-y$  plane and localized in the  $z$  direction, Eq. (C1) can be written as:

$$G_s(\mathbf{k}_{\parallel}, \omega) = G_0(\mathbf{k}_{\parallel}, \omega; 0) + G_0(\mathbf{k}_{\parallel}, \omega; 1)V(-1, 0)G_s(\mathbf{k}_{\parallel}, \omega), \quad (\text{C2})$$

where  $G_0(\mathbf{k}_{\parallel}, \omega; l)$  ( $l$  is an integer labelling the primitive cells in the  $z$  direction) is the bulk Green's function defined in the hybrid Wannier function basis:

$$G_0(\mathbf{k}_{\parallel}, \omega; l) = \int \frac{dk_z}{2\pi} e^{ik_z l} G_0(\mathbf{k}, \omega), \quad (\text{C3})$$

and the bulk Green's function  $G_0(\mathbf{k}, \omega)$  is:

$$G_0(\mathbf{k}, \omega) = \frac{-\tilde{\omega} \mathbb{I}_{2 \times 2} - (\tilde{t}_1 + t_2 \cos k_z) \tau_x - t_2 \sin k_z \tau_y}{\tilde{t}_1^2 + t_2^2 + 2\tilde{t}_1 t_2 \cos k_z - t_2^2 \tilde{\omega}^2}. \quad (\text{C4})$$

In the above equation  $\mathbb{I}_{2 \times 2}$  is the  $2 \times 2$  identity matrix,  $\tau_x, \tau_y$  and  $\tau_z$  are the Pauli matrices defined in the sublattice space.  $\tilde{t}_1$  and  $\tilde{\omega}$  are defined in Eq. (2) in Sec. III. If the bulk tight-binding model introduced in Sec. I is truncated at sublattice  $A$  with an ideal surface termination, the surface perturbation potential  $V(-1, 0)$  can be expressed as

$$V(-1, 0) = \begin{pmatrix} 0 & 0 \\ -t_2 & 0 \end{pmatrix}. \quad (\text{C5})$$

Plugging Eq. (C3)-(C5) into Eq. (C2), one obtains:

$$G_s(\mathbf{k}_{\parallel}, \omega)_{1,1} = \frac{G_0(\mathbf{k}_{\parallel}, \omega; 0)_{1,1}}{1 + t_2 G_0(\mathbf{k}_{\parallel}, \omega; 1)_{1,2}}. \quad (\text{C6})$$

where

$$G_0(\mathbf{k}_{\parallel}, \omega; 1)_{1,2} = - \int_{k_z} e^{ik_z} \frac{\tilde{t}_1 + t_2 e^{-ik_z}}{\tilde{t}_1^2 + t_2^2 + 2\tilde{t}_1 t_2 \cos k_z - t_2^2 \tilde{\omega}^2}, \quad (\text{C7})$$

and

$$G_0(\mathbf{k}_{\parallel}, \omega; 0)_{1,1} = \int_{k_z} \frac{-t_2 \tilde{\omega}}{\tilde{t}_1^2 + t_2^2 + 2\tilde{t}_1 t_2 \cos k_z - t_2^2 \tilde{\omega}^2}, \quad (\text{C8})$$

where  $\int_{k_z} = \int_0^{2\pi} dk_z / (2\pi)$ . Again,  $\tilde{\omega}$  is defined in Eq. (2). Defining  $\eta = e^{ik_z}$ , the integral over  $k_z$  in Eq. (C7) can be replaced by an contour integral around a unit circle in the complex plane of  $\eta$ , and can be solved exactly:

$$G_0(\mathbf{k}_{\parallel}, \omega; 1)_{1,2} = - \frac{\tilde{t}_1 \eta_+ + t_2}{\tilde{t}_1 t_2 (\sqrt{\gamma^2 - 4})}, \quad (\text{C9})$$

and

$$G_0(\mathbf{k}_{\parallel}, \omega; 0)_{1,1} = - \frac{t_2 \tilde{\omega}}{\tilde{t}_1 t_2 \sqrt{\gamma^2 - 4}}, \quad (\text{C10})$$

where

$$\gamma = (\tilde{t}_1^2 + t_2^2 - t_2^2 \tilde{\omega}^2) / (\tilde{t}_1 t_2), \quad (\text{C11})$$

and

$$\eta_+ = (-\gamma + \sqrt{\gamma^2 - 4}) / 2. \quad (\text{C12})$$

From Eq. (C9) one may notice that  $G_0(\mathbf{k}_{\parallel}, \omega; 1)_{1,2}$  is real only if  $\gamma^2 - 4 > 0$ , which implies that  $G_s(\mathbf{k}_{\parallel}, \omega)_{1,1}$  may have a pole on the real axis only when  $\gamma^2 - 4 > 0$ . It follows that  $\gamma^2 - 4 = 0$  defines the bulk spectral edge: when  $\gamma^2 - 4 < 0$ ,  $\omega$  is in the bulk continuum; while when  $\gamma^2 - 4 > 0$ ,  $\omega$  is in the bulk gap and there may be bound-state solutions. Then it is straightforward to show that:

$$\begin{cases} \text{if } -|k_{\parallel}^2 - k_0^2| < \tilde{\omega} < |k_{\parallel}^2 - k_0^2|, & \omega \text{ in the bulk gap,} \\ \text{if } \tilde{\omega} > |k_{\parallel}^2 - k_0^2| \text{ or } \tilde{\omega} < -|k_{\parallel}^2 - k_0^2|, & \omega \text{ in the bulk continuum,} \end{cases} \quad (\text{C13})$$

where  $k_0$  characterizing the size of the nodal loop is defined in Eq. (4), and  $\tilde{\omega}$  is defined in Eq. (2).

Plugging Eq. (C9) and Eq. (C10) into Eq. (C6), we obtain:

$$G_s(\mathbf{k}_{\parallel}, \omega) = \frac{-\tilde{\omega}}{\tilde{t}_1} \frac{1}{(\sqrt{\gamma^2 - 4} + \gamma)/2 - t_2/\tilde{t}_1}. \quad (\text{C14})$$

Plugging  $\tilde{t}_1 = t_2(1 + k_{\parallel}^2 - k_0^2)$  into Eq. (C11), considering the low-energy excitations around the nodal loop so that  $k_{\parallel}^2 - k_0^2$  and  $\tilde{\omega}$  are small, one obtains the final expression of the surface Green's function shown in Eq. (1) by dropping some terms higher order in  $k_{\parallel}^2 - k_0^2$  and  $\tilde{\omega}$ .

When  $\omega$  is in the bulk gap, Eq. (1) can be re-expressed as:

$$\begin{aligned} G_s(k_{\parallel}, \omega) &= \frac{-\tilde{\omega}}{t_2} \frac{1}{(\sqrt{(k_{\parallel}^2 - k_0^2)^2 - \tilde{\omega}^2} + k_{\parallel}^2 - k_0^2)} \\ &\approx \frac{-\tilde{\omega}}{t_2} \frac{1}{(|k_{\parallel}^2 - k_0^2| (1 - \tilde{\omega}^2 / (k_{\parallel}^2 - k_0^2)^2) + k_{\parallel}^2 - k_0^2)} \end{aligned} \quad (\text{C15})$$

From the above equation we see that for  $k_{\parallel} < k_0$ ,

$$G_s(k_{\parallel}, \omega) \approx \frac{(k_0^2 - k_{\parallel}^2)}{t_2 \tilde{\omega}}, \quad (\text{C16})$$

corresponding to the drumhead surface states at  $\tilde{\omega} = 0$ .

From the above analysis we see that when the surface is terminated at sublattice  $A$  there are drumhead surface states with dispersion  $t_0(k_{\parallel}^2 - k_0^2)$  inside the projected nodal loop. On the other hand, when the surface is terminated at sublattice  $B$ , the role of  $\tilde{t}_1$  and  $t_2$  is interchanged, so that there are drumhead surface states only when  $\tilde{t}_1 > t_2$ , i.e., outside the projected nodal loop ( $k_{\parallel} > k_0$ ). This explains the termination-dependent surface states as shown in Fig. 2(a)-(b).

## Appendix D: Derivations of surface dynamical susceptibility

### 1. Derivations of Eq. (12), Eq. (13)

We first derive the low-energy, long-wavelength behavior of the surface dynamical susceptibility of a hole-doped NLSM contributed by the extended bulk states projected at the surface, which are expressed by Eq. (12) and Eq. (13) in Sec. III. Such contributions are labelled as “ $b - b$ ” in Fig. (5)(a). In principle we need to calculate the imaginary part of  $\chi_{bb}(\mathbf{q}_{\parallel}, \nu, \mu)$  which is expressed in Eq. (11).

Again, we consider the situation that the nodal loop is centered at  $(\pi, \pi, \pi)$  whose size is small compared to the BZ. Then we expand  $\tilde{t}_1$  around  $(\pi, \pi)$  up to quadratic order of  $k_{\parallel}$  as shown in Eq. (3). Since we are interested in Fermi-surface fluctuations from the bulk continuum, we neglect the dispersion from  $t_0$ , so the spectral density of the bulk continuum  $f_b$  becomes

$$f_b(\mathbf{k}_{\parallel}, \epsilon) \approx \frac{\sqrt{\epsilon^2 - x_{\mathbf{k}_{\parallel}}^2}}{\epsilon} \theta(|\epsilon| - |x_{\mathbf{k}_{\parallel}}|). \quad (\text{D1})$$

Without loss of generality, the Bosonic wavevector  $\mathbf{q}_{\parallel}$  is chosen to point along the  $x$  direction,  $\mathbf{q}_{\parallel} = (q_{\parallel}, 0)$ . Then we define

$$x_{\mathbf{k}_{\parallel}} = k_{\parallel}^2 - k_0^2. \quad (\text{D2})$$

We also define

$$\begin{aligned} \tilde{\mu} &= \mu/t_2, \\ \tilde{\nu} &= \nu/t_2 \\ \tilde{t}_0 &= t_0/t_2. \end{aligned} \quad (\text{D3})$$

Plugging the expression of  $f_b$  in Eq. (D1) into Eq. (11), one obtains:

$$\begin{aligned}
\text{Im } \chi(\mathbf{q}_{\parallel}, \nu, \mu) &= \int_{\mathbf{k}_{\parallel}} \int_{-\tilde{\mu}}^{-\tilde{\mu}+\tilde{\nu}} d\epsilon \frac{\sqrt{\epsilon^2 - x_{\mathbf{k}_{\parallel}}^2} \sqrt{(\tilde{\nu} - \epsilon)^2 - x_{\mathbf{k}_{\parallel} + \mathbf{q}_{\parallel}}^2}}{-\epsilon(\tilde{\nu} - \epsilon)} \theta(|\epsilon| - |x_{\mathbf{k}_{\parallel}}|) \theta(|\nu - \epsilon| - |x_{\mathbf{k}_{\parallel} + \mathbf{q}_{\parallel}}|) \\
&= \int_{-\tilde{\mu}}^{-\tilde{\mu}+\tilde{\nu}} d\epsilon \int_{-\epsilon}^{\epsilon} dx \int_{-(\epsilon-\tilde{\nu})/(2k_0q_{\parallel})}^{(\epsilon-\tilde{\nu})/(2k_0q_{\parallel})} dy \frac{2k_0q_{\parallel} \sqrt{\epsilon^2 - x^2} \sqrt{(\tilde{\nu} - \epsilon)^2/(4k_0^2q_{\parallel}^2) - y^2}}{-\epsilon(\tilde{\nu} - \epsilon) \sqrt{1 - (y - (x + q_{\parallel}^2)/(2k_0q_{\parallel}))^2}} \\
&\approx \int_{-\tilde{\mu}}^{-\tilde{\mu}+\tilde{\nu}} d\epsilon \int_{-\epsilon}^{\epsilon} dx \int_{-(\epsilon-\tilde{\nu})/(2k_0q_{\parallel})}^{(\epsilon-\tilde{\nu})/(2k_0q_{\parallel})} dy \frac{2k_0q_{\parallel} \sqrt{\epsilon^2 - x^2} \sqrt{(\tilde{\nu} - \epsilon)^2/(4k_0^2q_{\parallel}^2) - y^2}}{-\epsilon(\tilde{\nu} - \epsilon)} \\
&= \int_{-\tilde{\mu}}^{-\tilde{\mu}+\tilde{\nu}} d\epsilon \int_{-\epsilon}^{\epsilon} dx \frac{\sqrt{\epsilon^2 - x^2} (\epsilon - \tilde{\nu})}{2k_0q_{\parallel} \epsilon} \\
&= \int_{-\tilde{\mu}}^{-\tilde{\mu}+\tilde{\nu}} d\epsilon \frac{\epsilon(\epsilon - \tilde{\nu})}{2k_0q_{\parallel}} \int_{-1}^1 dx' \sqrt{1 - x'^2} \\
&= \frac{\pi}{4k_0q_{\parallel}} (\epsilon^3/3 - \tilde{\nu}\epsilon^2/2) \Big|_{-\tilde{\mu}}^{-\tilde{\mu}+\tilde{\nu}} \\
&= \frac{\pi}{4k_0q_{\parallel}} (\tilde{\mu}^2\tilde{\nu} - \tilde{\nu}^3/6), \tag{D4}
\end{aligned}$$

where the second line of the above equation follows due to the heaviside  $\theta$  function, and  $y = (x + q_{\parallel}^2)/(2k_0q_{\parallel}) + \cos \phi$ , with  $\phi$  being the angle between  $\mathbf{k}_{\parallel}$  and  $\mathbf{q}_{\parallel}$ . We have made the approximation that  $\sqrt{1 - (y - (x + q_{\parallel}^2)/(2k_0q_{\parallel}))^2} \approx 1$  when going from the second to the third line in Eq. (D4). The fourth line of Eq. (D4) follows by using the integral identity:

$$\int_{-b}^b dy \sqrt{b^2 - y^2} = \frac{\pi}{2} b^2, \tag{D5}$$

where  $b = (\epsilon - \tilde{\nu})/(2k_0q_{\parallel})$ . Finally in the fifth line we define  $\epsilon x' = x$ , and it follows that  $\text{Im } \chi_{bb}(\mathbf{q}_{\parallel}, \nu, \mu) \sim \nu/q_{\parallel}$ . Eq. (12) is proved.

As discussed in the main text, the surface susceptibility is nonvanishing even at  $\mathbf{q}_{\parallel} = 0$  due to the bulk fluctuations. As expressed in Eq. (13),  $\text{Im } \chi(q_{\parallel} = 0, \nu, \mu) \sim \nu$  for  $\mu < 0$ . Using some similar tricks as those in Eq. (D4), it is straightforward to show that when  $q_{\parallel} = 0$ ,

$$\begin{aligned}
\text{Im } \chi(q_{\parallel} = 0, \nu, \mu) &= 2\pi \int_{-\tilde{\mu}}^{-\tilde{\mu}+\tilde{\nu}} d\epsilon \int_{-1}^1 dx' (\epsilon - \tilde{\nu}) \sqrt{1 - x'^2} \sqrt{1 - (1 - \tilde{\nu}/\epsilon)^2 x'^2} \\
&\approx \frac{4}{3} \pi (|\tilde{\mu}| \tilde{\nu} - \tilde{\nu}^2/2), \tag{D6}
\end{aligned}$$

where the integral over  $x'$  is approximated by a constant  $2/3$ . Such an approximation is valid as long as the frequency is much smaller than the Fermi level, i.e.,  $\nu \ll |\mu|$ . Thus Eq. (13) is proved.

## 2. Derivations of Eq. (15)-(16)

Now we turn to the case of Fig. 5(b), i.e., the surface bands are filled and the electron-hole excitations are mostly contributed by the  $b-b$  and  $s-b$  process.

Let us first consider the  $b-b$  process. Since we are interested in the bulk-state fluctuations, we neglect the dispersions from

$t_0$  in the bulk continuum spectral density, i.e.,  $\tilde{\omega} \approx \omega/t_2$ , and Eq. (D1) applies. One may still use Eq. (D4), except that now the Fermi level is right at the nodal energy  $\mu = 0$ . Then it immediately follows from Eq. (D4) that  $\text{Im } \chi(\mathbf{q}_{\parallel}, \nu, \mu = 0) \sim \nu^3/q_{\parallel}$ , which proves Eq. (15).

Next we consider the process that an electron is created in the bulk conduction band and a hole is left in the otherwise occupied surface bands as denoted by  $s-b$  in Fig. (5)(b). Let us consider a simplified case that  $t_0 = 0$  so that the surface

bands are perfectly flat and completely occupied. Then,

$$\begin{aligned} f_b(\mathbf{k}_{\parallel}, \epsilon) &\approx \frac{\sqrt{\epsilon^2 - x_{k_{\parallel}}^2}}{\epsilon} \theta(|\epsilon| - |x_{k_{\parallel}}|), \\ f_s(\mathbf{k}_{\parallel}, \epsilon) &\approx |x_{k_{\parallel}}| \delta(\epsilon) \theta(-x_{k_{\parallel}}). \end{aligned} \quad (\text{D7})$$

Plugging the above equation into Eq. (16), one obtains:

$$\begin{aligned} \text{Im } \chi_{\text{sb}}(\mathbf{q}_{\parallel}, \nu, \mu=0) &= \int_{\mathbf{k}_{\parallel}} \int_0^{\tilde{\nu}} d\epsilon f_s(-\epsilon, \mathbf{k}_{\parallel} - \mathbf{q}_{\parallel}) f_b(\tilde{\nu} - \epsilon, \mathbf{k}_{\parallel}) \\ &= \int_{\mathbf{k}_{\parallel}} \int_0^{\tilde{\nu}} d\epsilon |x_{\mathbf{k}_{\parallel} - \mathbf{q}_{\parallel}}| \delta(-\epsilon) \theta(-x_{\mathbf{k}_{\parallel} - \mathbf{q}_{\parallel}}) \frac{\sqrt{(\tilde{\nu} - \epsilon)^2 - x_{\mathbf{k}_{\parallel}}^2}}{\tilde{\nu} - \epsilon} \theta(|\tilde{\nu} - \epsilon| - |x_{\mathbf{k}_{\parallel}}|) \\ &\approx \int_{-\tilde{\nu}}^{\tilde{\nu}} dx \int_{(x+q_{\parallel}^2)/(2k_0 q_{\parallel})}^1 \frac{d \cos \phi}{\sqrt{1 - \cos^2 \phi}} (2q_{\parallel} \cos \phi \sqrt{k_0^2 + x - x - q_{\parallel}^2}) \frac{\sqrt{\tilde{\nu}^2 - x^2}}{\tilde{\nu}} \\ &= 2q_{\parallel} k_0 \int_{-\tilde{\nu}}^{\tilde{\nu}} dx \frac{\sqrt{\tilde{\nu}^2 - x^2}}{\tilde{\nu}} \sqrt{1 - (x + q_{\parallel}^2)^2 / (4k_0^2 q_{\parallel}^2)} - \int_{-\tilde{\nu}}^{\tilde{\nu}} \frac{\sqrt{\tilde{\nu}^2 - x^2}}{\tilde{\nu}} (x + q_{\parallel}^2) \int_{(x+q_{\parallel}^2)/(2k_0 q_{\parallel})}^1 \frac{d \cos \phi}{\sqrt{1 - \cos^2 \phi}} \\ &\approx 2q_{\parallel} k_0 \int_{-\tilde{\nu}}^{\tilde{\nu}} dx \frac{\sqrt{\tilde{\nu}^2 - x^2}}{\tilde{\nu}} \sqrt{1 - (x + q_{\parallel}^2)^2 / (4k_0^2 q_{\parallel}^2)} \\ &\approx 2q_{\parallel} k_0 \int_{-\tilde{\nu}}^{\tilde{\nu}} dx \frac{\sqrt{\tilde{\nu}^2 - x^2}}{\tilde{\nu}} \\ &= \pi k_0 q_{\parallel} \tilde{\nu}. \end{aligned} \quad (\text{D8})$$

In the above equation,  $x \equiv x_{\mathbf{k}_{\parallel}} = k_{\parallel}^2 - k_0^2$ , and we have made the approximation  $x_{\mathbf{k}_{\parallel} - \mathbf{q}_{\parallel}} = (|\mathbf{k}_{\parallel} - \mathbf{q}_{\parallel}|)^2 - k_0^2 \approx x + q_{\parallel}^2 - 2k_0 q_{\parallel} \cos \phi$ . We have used the integral identity,  $\int dx (1/\sqrt{1-x}) = -2\sqrt{1-x}$ , when going from the third to the fourth line; and we have dropped the second term on the right hand side of the fourth line because it is higher order  $\sim q_{\parallel}^2 \tilde{\nu}$  or  $\sim \tilde{\nu}^2 q_{\parallel}$ . Finally we have made the approximation

$\sqrt{1 - (x + q_{\parallel}^2)^2 / (4k_0^2 q_{\parallel}^2)} \approx 1$  from the fifth to the six line. We see that the final result presented in Eq. (D8) is consistent with Eq. (16) in the main text when  $t_0 = 0$ . It follows that when the  $\mu = 0$ , the  $s - b$  process dominate over the  $b - b$  process, and leads to a dynamical critical exponent  $z \approx 1$ .

Now we consider the case of nonvanishing  $t_0$ , i.e., the surface bands are not perfectly flat, but with a bandwidth  $\sim t_0$ . Plugging Eq. (8) into Eq. (16), then integrating over  $\epsilon$ , one obtains:

$$\text{Im } \chi_{\text{sb}}(\mathbf{q}_{\parallel}, \nu, \mu=0) = \int_{\mathbf{k}_{\parallel}} |x_{\mathbf{k}_{\parallel} - \mathbf{q}_{\parallel}}| \theta(-x_{\mathbf{k}_{\parallel} - \mathbf{q}_{\parallel}}) \theta(|\tilde{\nu} + \tilde{t}_0 x_{\mathbf{k}_{\parallel} - \mathbf{q}_{\parallel}}|) \frac{\sqrt{(\tilde{\nu} + \tilde{t}_0 x_{\mathbf{k}_{\parallel} - \mathbf{q}_{\parallel}})^2 - x_{\mathbf{k}_{\parallel}}^2}}{\tilde{\nu} + \tilde{t}_0 x_{\mathbf{k}_{\parallel} - \mathbf{q}_{\parallel}}}. \quad (\text{D9})$$

where  $x_{\mathbf{k}_{\parallel}}$  is defined in Eq. (D2). Let us define  $x \equiv x_{\mathbf{k}_{\parallel}}$  and  $y \equiv x_{\mathbf{k}_{\parallel} - \mathbf{q}_{\parallel}}$ . Since  $x$  is around 0, we make the following approximation to  $y$ :

$$\begin{aligned} y &= x_{\mathbf{k}_{\parallel} - \mathbf{q}_{\parallel}} \\ &= x - 2\sqrt{x^2 + k_0^2} q_{\parallel} \cos \phi + q_{\parallel}^2 \\ &\approx x - 2k_0 q_{\parallel} \cos \phi + q_{\parallel}^2. \end{aligned} \quad (\text{D10})$$

Plugging Eq. (D10) into Eq. (D9), and imposing the constraints on the limits of integrations from the two Heaviside  $\theta$  functions, one obtains

$$\begin{aligned} \text{Im } \chi_{\text{sb}}(\mathbf{q}_{\parallel}, \nu, \mu=0) &= \int_{x-2k_0q_{\parallel}+q_{\parallel}^2}^0 \frac{dy}{2k_0q_{\parallel}} \int_{-|\tilde{\nu}+\tilde{t}_0y|}^{|\tilde{\nu}+\tilde{t}_0y|} \sqrt{(\tilde{\nu}+\tilde{t}_0y)^2 - x^2} \frac{-y}{\tilde{\nu}+\tilde{t}_0y} \\ &\approx -\frac{\pi}{4k_0q_{\parallel}} \int_{-2k_0q_{\parallel}+q_{\parallel}^2}^0 dy y (\tilde{\nu}+\tilde{t}_0y), \end{aligned} \quad (\text{D11})$$

where the second line of the above equation follows due the following approximation on the limit of integration of  $y$ :

$$\int_{x-2k_0q_{\parallel}+q_{\parallel}^2}^0 \rightarrow \int_{-2k_0q_{\parallel}+q_{\parallel}^2}^0, \quad (\text{D12})$$

and we have used the integral identity

$$\int_{-|\tilde{\nu}+\tilde{t}_0y|}^{|\tilde{\nu}+\tilde{t}_0y|} dx \sqrt{(\tilde{\nu}+\tilde{t}_0y)^2 - x^2} = \frac{\pi(\tilde{\nu}+\tilde{t}_0y)^2}{2}. \quad (\text{D13})$$

Now we need to discuss two different situations:  $\tilde{\nu}+\tilde{t}_0y > 0$ , and  $\tilde{\nu}+\tilde{t}_0y < 0$ . If  $\tilde{\nu}+\tilde{t}_0y > 0$ , it follows from Eq. (D11) that

$$\text{Im } \chi_{\text{sb}}^>(\mathbf{q}_{\parallel}, \nu) = \frac{\pi\tilde{\nu}^3}{24k_0q_{\parallel}}. \quad (\text{D14})$$

If  $\tilde{\nu}+\tilde{t}_0y < 0$ , it turns out

$$\text{Im } \chi_{\text{sb}}^<(\mathbf{q}_{\parallel}, \nu) \approx -\frac{\pi\tilde{\nu}^3}{24k_0q_{\parallel}} + \frac{\pi k_0q_{\parallel}}{2}(\tilde{\nu} - \eta(t_0, q_{\parallel})). \quad (\text{D15})$$

Combining the above two equations,

$$\begin{aligned} \text{Im } \chi_{\text{sb}}(\mathbf{q}_{\parallel}, \nu) &= \text{Im } \chi_{\text{sb}}^<(\mathbf{q}_{\parallel}, \nu) + \text{Im } \chi_{\text{sb}}^>(\mathbf{q}_{\parallel}, \nu) \\ &= \frac{\pi k_0q_{\parallel}}{2}(\tilde{\nu} - \frac{2t_0}{3}(2k_0q_{\parallel} - q_{\parallel}^2)). \end{aligned} \quad (\text{D16})$$

Eq. (D16) has the same analytic behavior as Eq. (D8) when  $t_0 = 0$ , although the coefficients differ by a factor of 2. We attribute such a difference in the coefficients to the approximation shown in Eq. (D12), and we believe it is not important because it does not change the analytic behavior of  $\chi_{\text{sb}}$ .

It is also clearly seen from Eq. (D16) that the excitation gap  $\eta(t_0, q_{\parallel}) = 2t_0(2k_0q_{\parallel} - q_{\parallel}^2)/3$ , which is proportional to  $t_0$  and vanishes as  $q_{\parallel} \rightarrow 0$ . This is also in agreement with our numeric simulations as shown in Table. I.

#### Appendix E: Numeric calculations of surface dynamical susceptibility in slab geometry

In this section we explain the technical details in the numerical calculations of the surface dynamical susceptibility for a slab of NLSMs, as shown in Fig. 6 and Fig. 7. When both the surface Rashba SOC and Coulomb interactions are neglected, the system can be considered as spinless, and we use  $l, l'$  to label the lattice sites in the  $z$  direction in a slab of NLSMs. The matrix element of zero-temperature dynamical susceptibility is expressed as:

$$\chi_{ll'}(\mathbf{q}_{\parallel}, \nu) = i \int \frac{dk_x dk_y}{(2\pi)^2} \int \frac{d\omega}{2\pi} G_{ll'}^{(0)}(\mathbf{k}_{\parallel}, \omega) G_{ll'}^{(0)}(\mathbf{k}_{\parallel} + \mathbf{q}_{\parallel}, \omega + \nu), \quad (\text{E1})$$

where the  $G^{(0)}(\mathbf{k}_{\parallel}, \omega)$  is the noninteracting Green's function for a slab of NLSMs which can be expressed in matrix form as follows:

$$G^{(0)}(\mathbf{k}_{\parallel}, \omega) = V(\mathbf{k}_{\parallel}) G_{\text{diag}}^{(0)}(\mathbf{k}_{\parallel}, \omega) V^{\dagger}(\mathbf{k}_{\parallel}) \quad (\text{E2})$$

where  $G_{\text{diag}}^{(0)}$  is a  $2N \times 2N$  ( $N$  is the number of primitive cells in the slab, and there are two sublattices in each primitive cell) diagonal matrix whose  $j$ th diagonal element  $G_{\text{diag}}^{(0)}(\mathbf{k}_{\parallel}, \omega)_{jj} = 1/(\omega - \epsilon_j(\mathbf{k}_{\parallel}) + i\delta_{j,\mathbf{k}_{\parallel}})$ ,  $\delta_{j,\mathbf{k}_{\parallel}}$  is an infinitesimal quantity which is greater than (less than) 0 if the eigenenergy  $\epsilon_j(\mathbf{k}_{\parallel})$  is occupied (unoccupied).  $V(\mathbf{k}_{\parallel})$  is the eigenvector matrix of the Hamiltonian for the slab at  $\mathbf{k}_{\parallel}$  (denoted by  $H_{\text{slab}}(\mathbf{k}_{\parallel})$ ):  $\sum_{l'} H_{\text{slab}}(\mathbf{k}_{\parallel})_{ll'} V_{l',j}(\mathbf{k}_{\parallel}) = \epsilon_j(\mathbf{k}_{\parallel}) V_{l,j}(\mathbf{k}_{\parallel})$ . Then Eq. (E1) becomes

$$\chi_{ll'}(\mathbf{q}_{\parallel}, \nu) = i \int \frac{dk_x dk_y}{(2\pi)^2} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \sum_{j,j'=1}^{2N} \frac{W_{ll'jj'}(\mathbf{k}_{\parallel}, \mathbf{q}_{\parallel})}{(\omega - \epsilon_j(\mathbf{k}_{\parallel}) + i\delta_{j,\mathbf{k}_{\parallel}})(\omega + \nu - \epsilon_{j'}(\mathbf{k}_{\parallel} + \mathbf{q}_{\parallel}) + i\delta_{j',\mathbf{k}_{\parallel} + \mathbf{q}_{\parallel}})}, \quad (\text{E3})$$

where the spectral weight  $W_{ll'jj'}(\mathbf{k}_{\parallel}, \mathbf{q}_{\parallel})$  is defined as

$$W_{ll'jj'}(\mathbf{k}_{\parallel}, \mathbf{q}_{\parallel}) = V_{l',j}(\mathbf{k}_{\parallel}) V_{l,j}^*(\mathbf{k}_{\parallel}) V_{l',j'}(\mathbf{k}_{\parallel} + \mathbf{q}_{\parallel}) V_{l,j'}^*(\mathbf{k}_{\parallel} + \mathbf{q}_{\parallel}) \quad (\text{E4})$$

The integration over  $\omega$  can be carried out by closing the contour in the upper half plane, then Eq. (E3) becomes



$$\chi_{ll'}(\mathbf{q}_{\parallel}, \nu + i\delta) = \int \frac{dk_x dk_y}{(2\pi)^2} \sum_{j,j'=1}^{2N} \frac{W_{ll'jj'}(\mathbf{k}_{\parallel}, \mathbf{q}_{\parallel}) \left( \theta(\mu - \epsilon_j(\mathbf{k}_{\parallel})) - \theta(\mu - \epsilon_{j'}(\mathbf{k}_{\parallel} + \mathbf{q}_{\parallel})) \right)}{\epsilon_j'(\mathbf{k}_{\parallel} + \mathbf{q}_{\parallel}) - \epsilon_j(\mathbf{k}_{\parallel}) - \nu - i\delta} \quad (\text{E5})$$

If the top-surface layer is labelled as the 0th layer, then the surface susceptibility  $\chi_{\text{surf}}(\mathbf{q}_{\parallel}, \nu) = \chi_{00}(\mathbf{q}_{\parallel}, \nu)$ . The numeric integrations over  $k_x, k_y$  are replaced by discrete summations on a  $280 \times 280$   $\mathbf{k}$  mesh, and the infinitesimal quantity  $\delta$  is chosen as 0.001 in our numerical calculations. The number of primitive cells in the slab is 500.

### Appendix F: Bulk quantum oscillations

In this section we derive the dHvA quantum oscillations of bulk NLSMs neglecting Coulomb interactions. We consider two types of low-energy effective Hamiltonians of NLSMs as shown in Eq. (17). The energies of  $H_0^{\text{qua}}$  ( $H_0^{\text{lin}}$ ) in Eq. (17) have quadratic (linear) in-plane dispersions. The tight-binding model introduced in Sec. I can be reduced to a  $\mathbf{k} \cdot \mathbf{p}$  model around the center of the NLSM that is similar to  $H_0^{\text{qua}}$ ; the terms linear in  $\mathbf{k}_{\parallel}$  are killed by tetragonal symmetry. However, we would like to discuss both situations ( $H_0^{\text{qua}}$  and  $H_0^{\text{lin}}$ ) for the sake of generality.

Landau levels are formed when a magnetic field is applied along the  $z$  direction. The expressions of the Landau levels for  $H_0^{\text{qua}}$  and  $H_0^{\text{lin}}$  are shown in Eq. (18). As discussed in Sec. IV, the Landau levels become gapless whenever the nodal loop exactly overlaps with a quantized magnetic orbit. It is also mentioned that the gapless point there expects to be a sharp change in the free energy and the magnetic susceptibility show logarithmic divergence at zero temperature and zero Fermi level. In the remaining part of this section, we will explicitly derive the magnetic susceptibilities  $\chi(B)$  as expressed in Eq. (20)-(21).

The free energy of the Landau levels with chemical potential  $\mu$  is expressed as:

$$F = -\frac{eB}{\beta 2\pi^2 \hbar} \int_{-\pi}^{\pi} dk_z \sum_{n=0}^{\infty} \sum_{\lambda=\pm} \log(1 + e^{-(E_{\lambda}(n, k_z) - \mu)\beta}) \quad (\text{F1})$$

where the  $\lambda = \pm$  label the branch of Landau levels, and the Landau levels  $E_{\pm}(n, k_z)$  are expressed in Eq. (18) for both  $H_0^{\text{qua}}$  and  $H_0^{\text{lin}}$ . Summing over  $\lambda$ , Eq. (F1) becomes

$$F = -\frac{eB}{\beta 2\pi^2 \hbar} \int_{-\pi}^{\pi} dk_z \sum_{n=0}^{\infty} \log g(E(n, k_z), \mu, \beta), \quad (\text{F2})$$

where

$$g(E(n, k_z), \mu, \beta) = 1 + e^{-(E(n, k_z) - \mu)\beta} + e^{(E(n, k_z) + \mu)\beta} + e^{2\mu\beta}, \quad (\text{F3})$$

$E(n, k_z) = E_+(n, k_z)$  (see Eq. (18)), and  $\beta = 1/(k_B T)$ .

Then it is straightforward to calculate the magnetic suscep-

tibility  $\chi(B) = -\partial^2 F / \partial B^2$ :

$$\chi(B) = \frac{e}{2\pi^2 \hbar} \int_{-\pi}^{\pi} dk_z \sum_{n=0}^{\infty} (h_1 + h_2 + h_3) \quad (\text{F4})$$

where

$$\begin{aligned} h_1 &= h(E(n, k_z), \mu, \beta) \frac{\partial E(n, k_z)}{\partial B}, \\ h_2 &= B h(E(n, k_z), \mu, \beta) \frac{\partial^2 E(n, k_z)}{\partial^2 B}, \\ h_3 &= B \frac{\partial h(E(n, k_z), \mu, \beta)}{\partial E(n, k_z)} \left( \frac{\partial E(n, k_z)}{\partial B} \right)^2. \end{aligned} \quad (\text{F5})$$

$h(E(n, k_z), \mu, \beta)$  is defined as follows

$$h(E(n, k_z), \mu, \beta) = \frac{e^{(E(n, k_z) + \mu)\beta} - e^{-(E(n, k_z) - \mu)\beta}}{1 + e^{(E(n, k_z) + \mu)\beta} + e^{-(E(n, k_z) - \mu)\beta} + e^{2\mu\beta}}. \quad (\text{F6})$$

For NLSMs with quadratic in-plane dispersions, the Landau levels are defined in the first line of Eq. (18). Then the partial derivatives of  $E(n, k_z)$  with respect to  $B$  are readily obtained:

$$\begin{aligned} \frac{\partial E(n, k_z)}{\partial B} &= \frac{e(n + 1/2)(\omega_c(n + 1/2) - \Delta)}{m\sqrt{v^2 k_z^2 + (\Delta - \omega_c(n + 1/2))^2}}, \\ \frac{\partial^2 E(n, k_z)}{\partial^2 B} &= \frac{e(n + 1/2)^2 v^2 k_z^2}{m[v^2 k_z^2 + (\Delta - \omega_c(n + 1/2))^2]^{3/2}}. \end{aligned} \quad (\text{F7})$$

Plugging Eq. (F7) into Eq. (F4), one obtains that when  $\mu = 0$  and  $\beta \rightarrow \infty$  ( $T \rightarrow 0$ ), one obtains the expression of the magnetic susceptibility:

$$\begin{aligned} \chi(B) &= \frac{2e^2}{2\pi^2 \hbar m} \int_{-\pi}^{\pi} dk_z \sum_{n=0}^{\infty} \frac{(n + \frac{1}{2})(\omega_c(n + \frac{1}{2}) - \Delta)}{E(n, k_z)} \\ &\quad - \frac{e^2}{2\pi^2 \hbar m} \int_{-\pi}^{\pi} dk_z \sum_{n=0}^{\infty} (n + \frac{1}{2})^2 \frac{\omega_c}{E(n, k_z)}, \\ &\quad - \frac{e^2}{2\pi^2 \hbar m} \int_{-\pi}^{\pi} dk_z \sum_{n=0}^{\infty} (n + \frac{1}{2})^2 \frac{\omega_c(\omega_c(n + \frac{1}{2}) - \Delta)^2}{E(n, k_z)^3} \end{aligned} \quad (\text{F8})$$

The integration over  $k_z$  in Eq. (F8) can be carried out as follows:

$$\begin{aligned} \int_{-\pi}^{\pi} dk_z \frac{1}{E(n, k_z)} &= \frac{2}{v} \log \left( \frac{\sqrt{((n + \frac{1}{2}) - \frac{\Delta}{\omega_c})^2 + \Lambda^2 + \Lambda}}{|n + \frac{1}{2} - \frac{\Delta}{\omega_c}|} \right) \\ \int_{-\pi}^{\pi} dk_z \frac{1}{E(n, k_z)^3} &= \frac{2\Lambda}{v\omega_c^2(n + \frac{1}{2} - \frac{\Delta}{\omega_c})^2 \sqrt{(n + \frac{1}{2} - \frac{\Delta}{\omega_c})^2 + \Lambda^2}} \end{aligned} \quad (\text{F9})$$

where  $\Lambda = \pi v/\omega_c$  is a dimensionless cutoff parameter (the in-plane lattice parameter is set to unity).

Plugging Eq. (F9) into Eq. (F8), one obtains

$$\chi(B) = \frac{e^2 \omega_c}{2\pi^2 \hbar m} \sum_{n=0}^{\infty} \left( \left( n + \frac{1}{2} \right)^2 \frac{2}{v} \log(j(n, \omega_c, \Delta)) \right. \\ \left. + 2 \left( n + \frac{1}{2} \right) \left( n + \frac{1}{2} - \frac{\Delta}{\omega_c} \right) \frac{2}{v} \log(j(n, \omega_c, \Delta)) \right. \\ \left. - \left( n + \frac{1}{2} \right)^2 \frac{2\Lambda}{v \sqrt{(n + \frac{1}{2} - \frac{\Delta}{\omega_c})^2 + \Lambda^2}} \right), \quad (\text{F10})$$

where

$$j(n, \omega_c, \Delta) = \frac{\sqrt{((n + \frac{1}{2}) - \frac{\Delta}{\omega_c})^2 + \Lambda^2} + \Lambda}{|n + \frac{1}{2} - \frac{\Delta}{\omega_c}|} \quad (\text{F11})$$

The first term on the RHS of Eq. (F10) diverges logarithmically whenever  $\Delta/\omega_c \rightarrow (n + 1/2)$ . On the other hand, it is evidently seen that when  $\Delta = (n + 1/2)\omega_c$  is satisfied, the two Landau levels  $\pm E(n, k_z)$  become gapless at  $k_z = 0$ , and the size of the quantized magnetic orbit associated with the  $n$ th Landau level becomes exactly the same as the size of the nodal loop.

One may reproduce the above derivations for a NLSM with linear in-plane dispersions (see  $H_0^{\text{lin}}$  in Eq. (17)). It turns out that for linear in-plane dispersions, the magnetic susceptibility is expressed as

$$\chi(B) = \frac{eB}{2\pi^2 \hbar} \left( \frac{ev_0^2}{\omega_c} \right)^2 \sum_{n=0}^{\infty} \sqrt{n + \frac{1}{2}} \frac{\Delta}{\omega_c} \frac{2}{v} \log l(n, \omega_c, \Delta) \\ + \frac{e^2 v_0^2}{\pi^2 \hbar} \sum_{n=0}^{\infty} \sqrt{n + \frac{1}{2}} \left( \sqrt{n + \frac{1}{2}} - \frac{\Delta}{\omega_c} \right) \frac{2}{v} \log l(n, \omega_c, \Delta) \\ - \frac{eB}{2\pi^2 \hbar} \left( \frac{ev_0^2}{\omega_c} \right)^2 \sum_{n=0}^{\infty} \frac{2\Lambda(n + \frac{1}{2})}{v \omega_c^2 \sqrt{(\frac{\Delta}{\omega_c} - \sqrt{n + \frac{1}{2}})^2 + \Lambda^2}}, \quad (\text{F12})$$

where

$$l(n, \omega_c, \Delta) = \frac{\sqrt{(\frac{\Delta}{\omega_c} - \sqrt{n + \frac{1}{2}})^2 + \Lambda^2} + \Lambda}{|\frac{\Delta}{\omega_c} - \sqrt{n + \frac{1}{2}}|}. \quad (\text{F13})$$

The first term on the RHS of Eq. (F12) diverge logarithmically whenever  $\Delta = \omega_c \sqrt{n + 1/2}$ . Again, such a condition is exactly the gap-closure condition of Landau levels; in the meanwhile, the  $n$ th magnetic orbit exactly overlaps with the nodal loop when  $\Delta = \omega_c \sqrt{n + 1/2}$

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